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GENERALIZATION OF THE RAYLEIGH FORMULA TO THE MODEL WITH RING-SHAPED POTENTIALS

L. G. Mardoyan[1,2], A. N. Sissakian[3], V. M. Ter-Antonyan[1,2], T. A. Chatrchian[1]

[1] *Dep. of Physics, Yerevan State University 375049 Yerevan, Armenia*
[2] *Idjevan College-University, Idjevan, Armenia*
[3] *JINR Duna, 141980 Russia*

Abstract

The motion of a quantum particle is investigated in the ring-shaped model when the "bare" potential is equal to zero. Factorized in the spherical and cylindrical coordinates bases of this model are derived. The generalization of the Rayleigh expression for the plane wave expansion in the spherical waves is derived.

Formulation of the Problem.

Models with ring-sheped potentials are based on the Schrodinger operator with the potential part supplemented with the term $\Lambda/r^2\sin^2\theta$, where Λ is a nonnegative model parameter and θ is the angle between the axiz z and radius-vector of a particle. Thus, the ring-sheped models are models with a special axial symmetric addition to the "bare" potential. The most interesting are cases when "bare" potential is taken to be either a hydrogen atom (the Hartmann model [1-3]) or an isotropic oscillator (the Quesne model [4]). Recent intensive studies of these models have mainly dealt with bases and interbasis expansions in separable variables [5,6] and search for dynamic symmetries in the framework of ring-sheped potentials [7,8]. Note also that the Hartmann model has its origin in spectroscopic problems of the benzene molecule [3].

The aim of our paper is to investigate the free motion in the framework of ring-sheped potentials. We will derive wave functions of this model in terms of spherical and cylindrical coordinates and then will connect these bases by mens of an expansion that can be considering as a generalization of the Rayleigh expansion of the plane wave in spherical waves to the models with ring-sheped potentials.

General Information.

An arbitrary model with the ring-shaped potential is described by the equation ($\hbar = m = 1$):

$$\left(-\frac{1}{2}\Delta + U(r) + \frac{\Lambda}{r^2\sin^2\theta}\right)\Psi(\vec{r}) = E\Psi(\vec{r}) \tag{1}$$

where $U(r)$ is the central-symmetric "bare" potential.

It is known [9] that the solution of the equation (1) in spherical coordinates has the form

$$\Psi(r,\theta,\varphi;\delta) = R(r;\delta)Z_{lm}(\theta,\varphi;\delta)$$

where $\delta = \sqrt{m^2+2\Lambda} - |m|$, $R(r;\delta)$ is the solution of the radial equation, $Z_{lm}(\theta,\varphi;\delta)$ is a function which is convenient to call the ring-shaped (by analogy with the term "spherical function"). It is an eigenfunction of the operators $\hat{M} = \hat{l}^2 + 2\Lambda/\sin^2\theta$ and $\hat{l}_z$, namely

$$\begin{aligned}\hat{l}_z Z_{lm}(\theta,\varphi;\delta) &= mZ_{lm}(\theta,\varphi;\delta)\\ \hat{M}Z_{lm}(\theta,\varphi;\delta) &= (l+\delta)(l+\delta+1)Z_{lm}(\theta,\varphi;\delta)\end{aligned}$$

The explicit form of the $Z_{lm}(\theta,\varphi;\delta)$ function is given by expression

$$Z_{lm}(\theta,\varphi;\delta) = N_{lm}(\delta)(\sin\theta)^{|m|+\delta}\, C_{l-|m|}^{|m|+\delta+1/2}(\cos\theta)e^{im\varphi}$$

where $N_{lm}(\delta)$ is the normalization constant, and $C_n^{\nu}(x)$ are Gegenbauer polynomials:

$$C_n^{\nu}(x) = \frac{\Gamma(n+2\nu)}{\Gamma(2\nu)\Gamma(n+1)}{}_2F_1\left(-n, n+2\nu, \nu+\frac{1}{2}; \frac{1-x}{2}\right)$$

Under the normalization condition

$$\int Z^*_{l'm'}(\theta,\varphi;\delta)Z_{lm}(\theta,\varphi;\delta)d\Omega = \delta_{l'l}\delta_{m'm}$$

we have

$$N_{lm}(\delta) = (-1)^{\frac{m-|m|}{2}}2^{|m|+\delta}\Gamma\left(|m|+\delta+\frac{1}{2}\right)\left\{\frac{(2l+2\delta+1)(l-|m|)!}{4\pi^2\Gamma(l+|m|+2\delta+1)}\right\}^{\frac{1}{2}}$$

The representation for the $Z_{lm}(\theta,\varphi;\delta)$ function through the Rodrig's formula is valid too:

$$Z_{lm}(\theta,\varphi;\delta) = \frac{(-1)^{\frac{m+|m|}{2}}e^{i\pi\delta}e^{im\varphi}}{\Gamma(l+\delta+1)2^{l+\delta}}\left\{\frac{(2l+2\delta+1)\Gamma(l+|m|+2\delta+1)}{4\pi(l-|m|)!}\right\}^{\frac{1}{2}}\times$$

$$\times(\sin\theta)^{-|m|-\delta}\frac{d^{l-|m|}}{(d\cos\theta)^{l-|m|}}(\cos^2\theta-1)^{l+\delta} \qquad (2)$$

The information about the radial function $R(r;\delta)$ depends on the concrete form of the "bare" potential and is define of by the equation

$$\frac{d^2R}{dr^2}+\frac{2}{r}\frac{dR}{dr}+\left(k^2+U(r)-\frac{(l+\delta)(l+\delta+1)}{r^2}\right)R(r;\delta)=0$$

where $k=\sqrt{2E}$.

The Bases.

The free motion in the ring-shaped model is described by the equation

$$\left(-\frac{1}{2}\Delta+\frac{\Lambda}{r^2\sin^2\theta}\right)\Psi(\vec{r}) = E\Psi(\vec{r})$$

Let us consider the solution of this equation in the spherical and cylindrical coordinates. The radial equation in the spherical coordinates has the following form

$$\frac{d^2R}{dr^2}+\frac{2}{r}\frac{dR}{dr}+\left(k^2-\frac{(l+\delta)(l+\delta+1)}{r^2}\right)R(r;\delta)=0$$

The corresponding solution can be expressed via the Bessel function

$$R_{kl}(r;\delta) = \frac{C_{kl}(\delta)}{\sqrt{r}}J_{l+\delta+\frac{1}{2}}(kr)$$

Under the normalization codition

$$\int \Psi^*_{k'l'm'}(r,\theta,\varphi;\delta)\Psi_{klm}(r,\theta,\varphi;\delta)dV = 2\pi\delta(k-k')\delta_{ll'}\delta_{mm'}$$

$C_{kl}(\delta)=\sqrt{2\pi k}$. The asymptotics of the radial function $R_{kl}(\delta)$ for small and large r is given by the following relations:

$$R_{kl}(r,\delta) \xrightarrow{r\to 0} \frac{2k\Gamma(l+\delta+1)}{\Gamma(2l+2\delta+2)}(2kr)^{l+\delta}$$
$$R_{kl}(r,\delta) \xrightarrow{r\to\infty} \frac{2}{r}\sin\left[kr-\frac{\pi}{2}(l+\delta)\right]$$

These expressions go to the known results, if the parameter δ is equal zero.

So, we see that the spherical basis of the free motion in the ring-shaped model has the form

$$\Psi_{klm}(r,\theta,\varphi;\delta)=\sqrt{\frac{2\pi k}{r}}J_{l+\delta+\frac{1}{2}}(kr)Z_{lm}(\theta,\varphi;\delta) \tag{3}$$

When $\delta=0$, this result goes to the spherical wave.

In the cylindrical coordinates the scheme of separation of the variables corresponds to the factorization

$$\Phi(\rho,\varphi,z;\delta)=R(\rho;\delta)e^{ik_z z}\frac{e^{im\varphi}}{\sqrt{2\pi}}$$

which leads to the radial equation

$$\frac{d^2R}{d\rho^2}+\frac{1}{\rho}\frac{dR}{d\rho}+\left(\omega^2-\frac{(|m|+\delta)^2}{\rho^2}\right)R(\rho;\delta)=0 \tag{4}$$

where $\omega=\sqrt{k^2-k_z^2}$. The normalization condition is

$$\int \Phi^*_{\omega' k'_z m'}(\rho,\varphi,z;\delta)\Phi_{\omega k_z m}(\rho,\varphi,z;\delta)dV=4\pi^2\delta(\omega-\omega')\delta(k_z-k'_z)\delta_{mm'}$$

Then for the regular solution of the equation (4) we have the following representation in terms of the Bessel function:

$$R_{\omega m}(\rho;\delta)=\sqrt{2\pi\omega}J_{|m|+\delta}(\omega\rho)$$

This solution has the asymptotic form

$$R_{\omega m}(\rho;\delta)\xrightarrow{\rho\to\infty}\frac{2}{\sqrt{\rho}}\sin\left[\omega\rho-\frac{\pi}{2}\left(|m|+\delta-\frac{1}{2}\right)\right]$$

The cylindrical basis is

$$\Phi_{\omega k_z m}(\rho,\varphi,z;\delta)=\sqrt{\omega}J_{|m|+\delta}(\omega\rho)e^{ik_z z}e^{im\varphi}$$

In the following the notation are more convenient:

$$k_z=k\cos\gamma,\qquad \omega=k\sin\gamma,\qquad o\le\gamma\le\pi$$

in which

$$\Phi_{k\gamma m}(\rho,\varphi,z;\delta)=\sqrt{k\sin\gamma}J_{|m|+\delta}(k\rho\sin\gamma)e^{ikz\cos\gamma}e^{im\varphi} \tag{5}$$

Expansion.

Let us consider the expansion of the cylindrical basis over the spherical one. This expansion must have the form

$$\Phi_{k\gamma m}(\rho,\varphi,z;\delta)=\sum_{l=|m|}^{\infty}W_{lm}^{k\gamma}(\delta)\Psi_{klm}(r,\theta,\varphi;\delta) \tag{6}$$

Our purpose is to calculate the matrix $W_{lm}^{k\gamma}(\delta)$. The following steps must be executed for this purpose:

(a) substitute the expressions (3) and (5) into (6);

(b) multiply both the parts of the expansion (6) by $Z^*_{l'm}(\theta,\varphi;\delta)$, integrate over the solid angle and use the orthonormalization property of the ring-shaped function;

(c) use the expansions

$$J_{|m|+\delta}(k\rho\sin\gamma) = \sum_{s=0}^{\infty}\frac{(-1)^s\left(\frac{1}{2}k\rho\sin\gamma\right)^{|m|+\delta+2s}}{s!\,\Gamma(|m|+\delta+s+1)}$$
$$e^{ikz\cos\gamma} = \sum_{t=0}^{\infty}\frac{(ikz\cos\gamma)^t}{t!}$$

(d) go to the spherical coordinates from the cylindrical ones in the left part of the expansion (6).

Instead of (6), doing the mentioned steps we arrive of the expansion

$$W^{k\gamma}_{lm}(\delta)\sqrt{\frac{2\pi}{r}}J_{l+\delta+\frac{1}{2}}(kr) = \frac{\sqrt{\sin\gamma}}{\Gamma(|m|+\delta+1)}\sum_{s=0}^{\infty}\frac{(-1)^s\left(\frac{1}{2}k\sin\gamma\right)^{|m|+\delta+2s}}{s!\,(|m|+\delta+1)_s}\times$$
$$\times\sum_{t=0}^{\infty}\frac{(ik\cos\gamma)^t}{t!}r^{|m|+\delta+2s+t}Q^{lm}_{st}(\delta)$$

where

$$Q^{lm}_{st}(\delta) = \int(\cos\theta)^t(\sin\theta)^{2s+|m|+\delta}e^{im\varphi}Z^*_{lm}(\theta,\varphi;\delta)d\Omega$$

Using the expression (2) and subsequently integrate by parts we can be convinced that the $Q^{lm}_{st}(\delta)$ differs from zero only under the condition $2s+t+|m|-l\geq 0$. Thus, all members of the series contain r in nonnegative power of r, so as in the limit, when $r\to 0$, we obtain

$$W^{k\gamma}_{lm}(\delta) = i^{l-|m|}\sqrt{\frac{\sin\gamma}{\pi k}}\frac{\Gamma\left(l+\delta+\frac{3}{2}\right)}{\Gamma(|m|+\delta+1)}(2\cos\gamma)^{l-|m|}(\sin\gamma)^{|m|+\delta}\times$$
$$\times\sum_{s=0}^{\left[\frac{l-|m|}{2}\right]}\frac{\left(\frac{1}{4}\tan^2\gamma\right)^s}{s!(|m|+\delta+1)_s}\frac{Q^{lm}_{s,l-|m|-2s}(\delta)}{(l-|m|-2s)!} \tag{7}$$

where

$$\left[\frac{l-|m|}{2}\right] = \begin{cases}\frac{l-|m|}{2}, & l-|m|=2n;\\ \frac{l-|m|-1}{2}, & l-|m|=2n+1.\end{cases}$$

When $t=l-|m|-2s$ the expression for the $Q^{lm}_{st}(\delta)$ is easily integrated:

$$Q^{lm}_{s,l-|m|-2s}(\delta) = (-1)^{s+\frac{m-|m|}{2}}\frac{2^{l+\delta+1}\Gamma(l+\delta+1)}{\Gamma(2l+2\delta+2)}\times$$
$$\times\left\{\pi(2l+2\delta+1)(l-|m|)!\Gamma(l+|m|+2\delta+1)\right\}^{\frac{1}{2}}$$

If we substitute the last expression into (7) and use the formula

$$\Gamma(2z) = \frac{2^{2z-1}}{\sqrt{\pi}}\Gamma(z)\Gamma\left(z+\frac{1}{2}\right)$$

we obtain

$$W_{lm}^{k\gamma}(\delta) = (-1)^{\frac{m-|m|}{2}} i^{l-|m|} \left\{ \frac{\pi(2l+2\delta+1)\Gamma(l+|m|+2\delta+1)\sin\gamma}{k(l-|m|)!} \right\}^{\frac{1}{2}} \times$$

$$\times \frac{(\cos\gamma)^{l-|m|}(\sin\gamma)^{|m|+\delta}}{2^{|m|+\delta}\Gamma(|m|+\delta+1)} {}_2F_1\left(-\frac{l-|m|}{2}, -\frac{l-|m|-1}{2}, |m|+\delta+1; -\tan^2\gamma\right)$$

The matrix $W_{lm}^{k\gamma}(\delta)$ can also be expressed via the Gegenbauer polynomials. For this aim we should be use the expression which connects the hypergeometrical function of the argument z with the hypergeometrical function of the argument $1-z$:

$${}_2F_1(\alpha,\beta,\gamma;z) = \frac{\Gamma(\gamma)\Gamma(\gamma-\alpha-\beta)}{\Gamma(\gamma-\alpha)\Gamma(\gamma-\beta)} {}_2F_1(\alpha,\beta,\alpha+\beta+1-\gamma;1-z)+$$

$$+\frac{\Gamma(\gamma)\Gamma(\alpha+\beta-\gamma)}{\Gamma(\alpha)\Gamma(\beta)}(1-z)^{\gamma-\alpha-\beta} {}_2F_1(\gamma-\alpha,\gamma-\beta,\gamma+1-\alpha-\beta;1-z)$$

and the representation of the Gegenbauer polynomials over the hypergeometrical function

$$C_n^{\nu}(z) = \frac{(2z)^n\Gamma(\nu+n)}{n!\Gamma(\nu)} {}_2F_1\left(-\frac{n}{2}, \frac{1}{2}-\frac{n}{2}, 1-\nu-n; -z^2\right)$$

The final result has the form

$$W_{lm}^{k\gamma}(\delta) = (-1)^{\frac{m-|m|}{2}} i^{l-|m|} \Gamma\left(|m|+\delta+\frac{1}{2}\right) \left\{ \frac{(2l+2\delta+1)(l-|m|)!\sin\gamma}{k\Gamma(l+|m|+2\delta+1)} \right\}^{\frac{1}{2}} \times$$

$$\times(2\sin\gamma)^{|m|+\delta}\, C_{l-|m|}^{|m|+\delta+\frac{1}{2}}(\cos\gamma) \tag{8}$$

The expressions (6) and (8) define completely, in the free ring-shaped model the expansion of the cylindrical basis over spherical one.

It may easily be checked that when $m=\delta=\gamma=0$ the expansion (6) turns into the known Rayleigh's expansion for the plane wave over the spherical waves:

$$e^{ikz} = \sum_{l=0}^{\infty} \frac{i^l}{k}\sqrt{\pi(2l+1)}\, \Psi_{kl0}(r,\theta,\varphi)$$

Here

$$\Psi_{klm}(r,\theta,\varphi) = \sqrt{\frac{2\pi k}{r}}\, J_{l+\frac{1}{2}}(kr)Y_{lm}(\theta,\varphi)$$

The expansion (6) can be reduced to the form known in the theory of special functions. To verify that, we substitute the spherical and cylindrical bases into (6) and expression (8) then, turn to the spherical coordinates. We obtain the expression:

$$(kr\sin\theta\sin\gamma)^{-|m|-\delta} J_{|m|+\delta}(kr\sin\theta\sin\gamma)e^{ikr\cos\beta\cos\gamma} =$$

$$= \sqrt{2}(kr)^{-|m|-\delta-\frac{1}{2}}\Gamma\left(|m|+\delta+\frac{1}{2}\right) \times$$

$$\times \sum_{l=|m|}^{\infty} \frac{i^{l-|m|}\Gamma(2|m|+2\delta+1)\Gamma(l+\delta+\frac{1}{2})(l-|m|)!}{\Gamma(|m|+\delta+1)\Gamma(l+|m|+2\delta+1)} \times$$

$$\times J_{l+\delta+\frac{1}{2}}(kr) C_{l-|m|}^{|m|+\delta+\frac{1}{2}}(\cos\theta) C_{l-|m|}^{|m|+\delta+\frac{1}{2}}(\cos\gamma)$$

Let's introduce new notes

$$y = kr, \quad \lambda = |m| + \delta + \frac{1}{2}, \quad n = l - |m|$$

So, our result turns into the expression

$$(y \sin\theta \sin\gamma)^{\frac{1}{2}-\lambda} J_{\lambda-\frac{1}{2}}(y \sin\theta \sin\gamma) e^{iy\cos\theta\cos\gamma} =$$

$$= \sqrt{2} y^{-\lambda} \Gamma(\lambda) \sum_{n=0}^{\infty} i^n \frac{n!(n+\lambda)}{(2\lambda)_n \Gamma\left(\lambda + \frac{1}{2}\right)} J_{n+\lambda}(y) C_n^\lambda(\cos\theta) C_n^\lambda(\cos\gamma) \tag{9}$$

from the monograph [10]. Thus, firstly, we have convinced that our result is correct, secondly, we derived the connection of free the ring-shaped model with the concrete region of the theory of special functions. Remark additionally that for $\gamma = 0$ (9) turns into the expression from the monograph [10] also:

$$e^{ixy} = \Gamma(\lambda) \left(\frac{y}{2}\right)^{-\lambda} \sum_{n=0}^{\infty} i^n (n+\lambda) J_{n+\lambda}(y) C_n^\lambda(x)$$

Conclusion.

We have obtained the generalization of the known Rayleigh's expansion for the case of ring-shaped potentials. Since that result can be used for the construction of the corresponding phase scattering theory with the ring-shaped potentials, this expansion acquires a principal significance.

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